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Wave Functions and Finite Size Effects in a Two-Dimensional Lattice Field Theory†

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Abstract

A study of finite size corrections to the masses of fermions and bound states in the Baxter/ massive Thirring/ sine Gordon lattice field theory is discussed. It is shown that information on bound state wave functions may be used to extrapolate Monte Carlo mass calculations to infinite volume.

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Numerical lattice QCD calculations are often carried out inside a box whose physical size is, at best, only slightly larger than a hadron.[1] In this situation, the question of how large the box must be to have a negligible (or calculable) effect on the physics is an important consideration in selecting the parameters of the calculation. Recent work by Weingarten and Velikson[2] and by Gottlieb[3] has shown that the data generated in Monte Carlo investigations of the hadron spectrum can also be used to study hadron wave functions, which are extracted from correlation functions involving spatially extended operators. The results are quite reasonable and indicate, for example, that at $\beta=5.7$ ($a\approx0.2$ fermi) hadron wave functions fall off substantially with quark separations of 3 or 4 sites. In addition to the intrinsic interest of studying hadron wave functions, these results may also provide a very economical way of estimating finite size effects on spectrum calculations. The important practical point here is that, once the gauge configurations and quark propagators are generated for the spectrum calculations, the study of hadron wave functions requires a negligible amount of additional computer time. In contrast, a direct study of finite size effects by varying the size of the box is a very expensive proposition requiring independent simulations with very good statistics at several different box sizes. It would clearly be advantageous to avoid such a calculation by using the wave functions on a fixed size lattice to estimate finite size effects. To study this possibility David Hochberg and I carried out a Monte Carlo investigation[4] of the two-dimensional Baxter/ massive Thirring/ sine Gordon model.[5-9] This is a very convenient toy model for several reasons. It has a nontrivial spectrum consisting of fermions and an adjustable number of fermion-antifermion bound states (sine Gordon mesons). For an infinite volume lattice, the spectrum is exactly known for all lattice spacings (i.e. not just in the continuum limit).[8,9] One may also carry out Monte Carlo calculations of the spectrum and of the bound state wave functions which are quite analogous to the calculations in QCD. By exploiting the fact that the Baxter model is equivalent to the lattice massive Thirring model, we were able to carry out the Monte Carlo calculations in terms of the Ising-like spins $\sigma_{ij}=\pm 1$ of the Baxter model with an action consisting of local 2-spin and 4-spin couplings. The simplicity of the action combined with the fact that the model is two-dimensional enabled us to obtain very accurate Monte Carlo results (±3% for masses) with only a modest investment of computer time. It should be noted that the Baxter model constitutes an exact treatment of massive Thirring fermions[9] including closed loops, so there is no need for a "quenched" approximation.

To study the dynamics of finite size effects, we varied three different parameters in the calculation: (1) The size of the box in lattice units, i.e. the number of lattice sites in the space direction; (2) The infinite volume mass of the fermion in lattice units (this is determined by an elliptic modulus in the standard Baxter parametrization of the spin couplings[8]); (3) The coupling constant g which controls the strength of the Thirring interaction (and also determines the bound state masses). The spatial size of the lattice varied from 6 to 100 sites. The number of sites in the time direction was always taken to be ≥30, long enough to see pure exponential time-dependence for Fourier transformed correlation functions over a large range of time separations. For an infinite volume lattice, the fermion and bound state masses are given in terms of the Baxter couplings by analytic formulas involving elliptic functions. These were first derived in Ref. 8 and are summarized in Ref. 4. In the Monte Carlo calculation, the mass of the fermion m_F was extracted from the spin-spin correlation function (for $T>T_c$), while the mass of the lowest lying bound state m_B was obtained from the correlation function for composite operators constructed from nearest-neighbor spin pairs $\sigma_{i,j}\sigma_{i+1,j}$ separated by one site in the spatial direction. The latter operator corresponds to $\bar{\psi}\gamma_5\psi$ in the fermion representation. Thus, we looked at the long range behavior of the functions

$$F(\tau) = \sum_x \langle\sigma_{0,0}\sigma_{x,\tau}\rangle \sim Z_F(e^{-m_F\tau} + e^{-m_F(N_t-\tau)}) \tag{1}$$

$$B(\tau) = \sum_x \langle\sigma_{0,0}\sigma_{1,0}\sigma_{x,\tau}\sigma_{x+1,\tau}\rangle \sim Z_B(e^{-m_B\tau} + e^{-m_B(N_t-\tau)}) \tag{2}$$

where N_t is the length of the lattice in the time direction. The bound state wave function $\Psi(y)$ was extracted from the correlation function between a nearst neighbor spin pair and a spatially extended spin pair,

$$B(\tau;y) = \sum_x \langle\sigma_{0,0}\sigma_{1,0}\sigma_{x,\tau}\sigma_{x+y,\tau}\rangle \sim Z_B\Psi(y)(e^{-m_B\tau} + e^{-m_B(N_t-\tau)}) \tag{3}$$

with y odd. It is a nontrivial test of this method that the exponent m_B in (3) is the same as that in (2). We found this to be true to very high accuracy. The coefficient $Z_B\Psi(y)=Z_B^{\frac{1}{2}}\times Z_B^{\frac{1}{2}}\Psi(y)$ represents the factorized residue of the bound-state pole, so that $Z_B^{\frac{1}{2}}\Psi(y)$ is the vacuum-to-bound-state matrix element of the spatially extended operator.

We began by considering the Ising/free-fermion case of the Baxter model ($g=0$ or in conventional Baxter model notation $\mu=\pi/2$ where $g=-2\cot\mu$). In this case, the spectrum consists of only the fermion. The Monte Carlo results for the spin-spin correlation function on a 30×30 lattice are shown in Fig. 1 along with the exponential fit defined in Eq. (1). Note the extremely high quality of the exponential fit over a large number of sites. This was typical of all the correlation functions we measured, including those for nonlocal operators, which made the task of extracting masses and wave functions quite straightforward and unambiguous. The mass of the fermion in the free field case is shown for various box sizes in Fig. 2. The infinite volume fermion mass was chosen to be $m_{F\infty}=0.1178$, which corresponds to a Compton wavelength (spin-spin correlation length) of about $8\frac{1}{2}$ sites. We see that the shift of the mass due to finite size effects is positive and monotonically increasing as the box size is decreased. The shift becomes large when the box is approximately twice the Compton wavelength of the fermion. The solid curve in Fig. 2 is an empirical fit given by

$$m_F = \left(m_{F\infty}^2 + \frac{0.93}{L^2}\right)^{1/2} \tag{4}$$

It should be noted that the Jordan-Wigner transformation between spins and fermions in a finite volume involves boundary terms (c.f. Ref. 10) which shift the allowed momenta by $O(1/L)$. This might explain the form of Eq. (4). [Our lattice is periodic in the spin variables, i.e. in the language of Ref. 10 we treat the "a-cyclic" problem rather than the "c-cyclic" problem.]

Next we considered the more interesting case of the interacting theory. We took $\mu=0.65\pi$ corresponding to the weakly attractive coupling region in which there is a single fermion-antifermion bound state. [In general, there are n bound states for $(\frac{n}{n+1})\pi<\mu<(\frac{n+1}{n+2})\pi$.] Taking the fermion mass $m_{F\infty}=0.1178$ as before, the infinite volume bound state mass is $m_{B\infty}=0.1762$. The Monte Carlo results for the fermion and bound state masses on lattices of spatial dimension 100, 50, 30, 20, 10, and 6 sites are shown in Fig. 3. The fermion is close to its infinite volume value for $L\approx30$, dips slightly at $L=20$ and then increases rapidly for smaller lattices in a manner similar to the free fermion case. In contrast, the bound state mass is noticeably below $m_{B\infty}$ even for $L=50$ and is more than 20% low for $L=20$. For very small lattices, the bound state mass turns around and begins to increase rapidly, apparently in unison with the fermion mass.

The rest of our Monte Carlo calculations were devoted to understanding the bound state mass curve in Fig. 3. We found that this curve is the result of two competing effects. The large positive mass shift of the bound state for very small lattices is a result of the increasing mass of its fermion constituents. The size scale at which this effect becomes relevant is roughly $2m_F^{-1}\approx17$ sites. To verify this interpretation, we increased the fermion mass to $m_{F\infty}=0.2043$ or $2m_F^{-1}\approx10$ sites. For lattices down to $L=10$, the fermion mass was essentially equal to its infinite volume value while the bound state mass was monotonically decreasing with no tendency to turn upward (see Ref. 4 for details), thus confirming the idea that the relevant length scale for the positive component of the mass shift is the fermion Compton wavelength.

The other finite size effect exhibited by the bound state mass curve in Fig. 3 is a negative mass shift for lattices of moderate size. We found that the box size at which this effect becomes relevant is determined by the spatial extent of the bound state wave function. We looked at wave functions on a 30×30 lattice for three different values of the coupling constant: $\mu = 0.65\pi$, 0.72π, and 0.83π ($g = 1.02$, 1.76, and 3.15 respectively). The Monte Carlo results for the square of the wave function $\Psi(y)$, which were extracted from the correlation functions (3), are shown in Fig. 4. The theoretical infinite volume bound state mass was held fixed at $m_{B\infty}=0.1762$. The measured values of the mass on a 30×30 lattice were $m_B=.1348\pm.0024$, $.1548\pm.0042$, and $.1751\pm.0050$ for $\mu=.65\pi$, $.73\pi$, and $.82\pi$ respectively. Note that as we increase the coupling and pull in the wave function to a smaller size, the mass approaches the correct infinite volume value. For the strongest of the three couplings, $.82\pi$, the wave function is quite well contained in the 30 site box, and correspondingly, we see no finite size correction to the mass ($m_B \approx m_{B\infty}$ within errors). In fact, the mass correction in all cases appears to be roughly proportional to $|\Psi(L/2)|^2$, i.e. the squared wave function at maximum separation on the periodic lattice. Returning to the bound state mass curve in Fig. 3, we find that a very good description of the finite size effects for $L>30$ is given by

$$m_B = m_{B\infty} + c\ |\Psi(L/2)|^2 \tag{5}$$

This gives the solid curve in Fig. 3. In Eq. (5) we measured the wave function for each value of L directly, using a lattice of length L. However, these values could have been quite accurately estimated using only the data from the 30 site lattice by simply fitting the tail of the wave function to a periodic exponential (analogous to the right hand side of (1)) and extrapolating. Similarly, we might use Eq. (5) to define a procedure for extrapolating to infinite volume by measuring the mass and wave functions for two values of L and solving for $m_{B\infty}$ and c. For example, if we use the data for L=30 and 50 we obtain the extrapolated value $m_{B\infty}$=.1771±.005 which is actually somewhat closer to the correct infinite volume value (.1762) than the result we obtained from a direct calculation on a 100×100 lattice.

Some of our results may have implications for QCD spectrum calculations (particularly those including closed loops, which is presently only feasible on rather small lattices). The formula (5) might have an analog for QCD bound states. [Presumably, in three space dimensions, $|\Psi(L/2)|^2$ should be replaced by an integral of $|\Psi|^2$ over the surface of a cube.] It would then be possible to do spectrum calculations on moderate size lattices and correct for finite size effects by calculating hadron wave functions.

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FIGURE CAPTIONS

Fig. 1: Spin-spin correlation function on a 30×30 lattice with $\mu = .50\pi$ (free fermions) and $m_{F\infty} = 0.1178$. The solid line is the fit defined in Eq. (1).

Fig. 2: The fermion mass as a function of lattice size with $\mu = .50\pi$ (free fermions) and $m_{F\infty} = 0.1178$. The solid line is the fit defined in Eq. (4).

Fig. 3: The fermion and bound state mass as a function of lattice size for $m_{F\infty} = 0.1178$ and $m_{B\infty} = 0.1762$ ($\mu = .65\pi$). The dashed lines are to guide the eye. The solid curve is a calculation of the finite size correction to the bound state mass from Eq. (5).

Fig. 4: Squared wave functions for three values of the coupling constant.

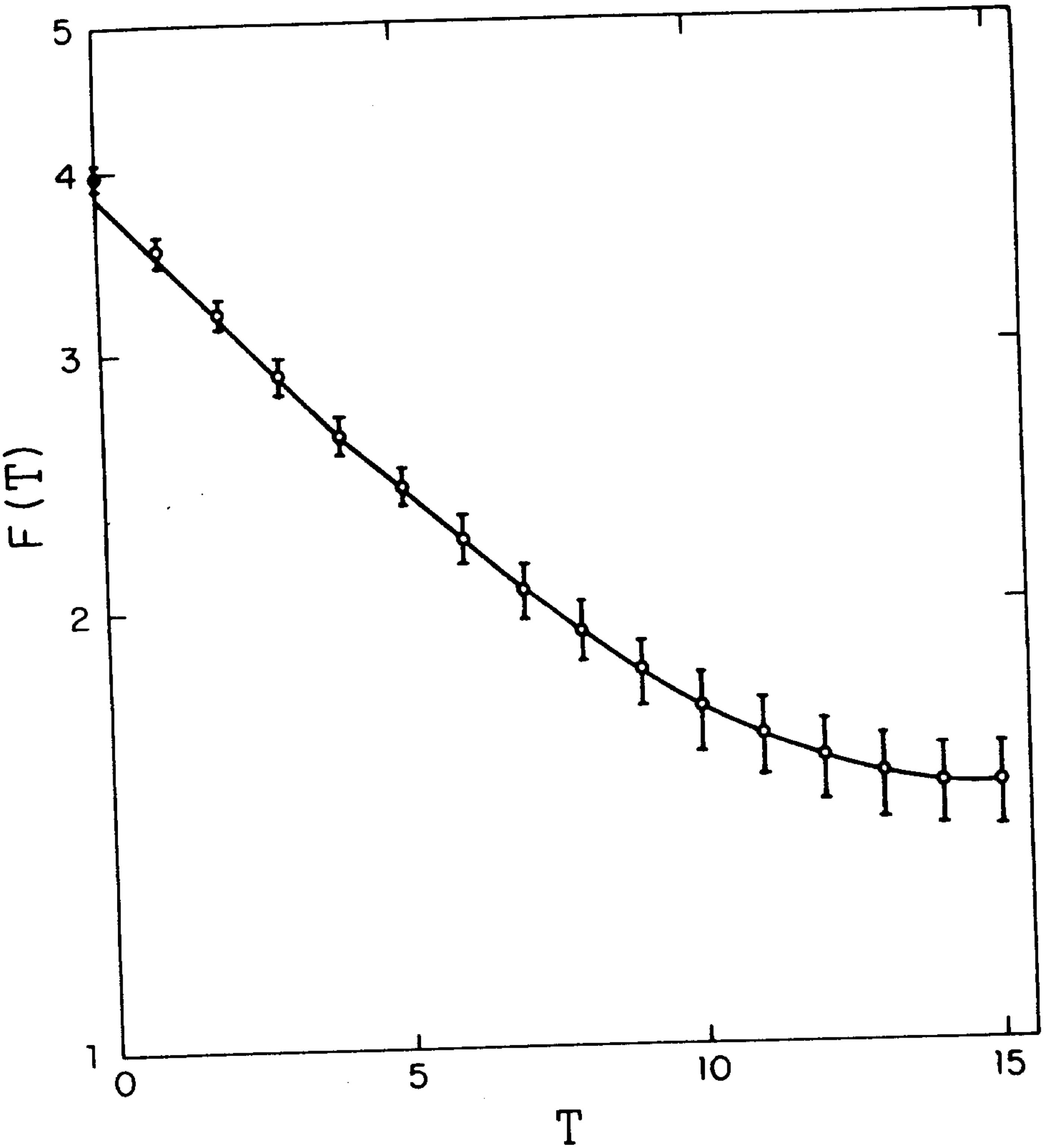
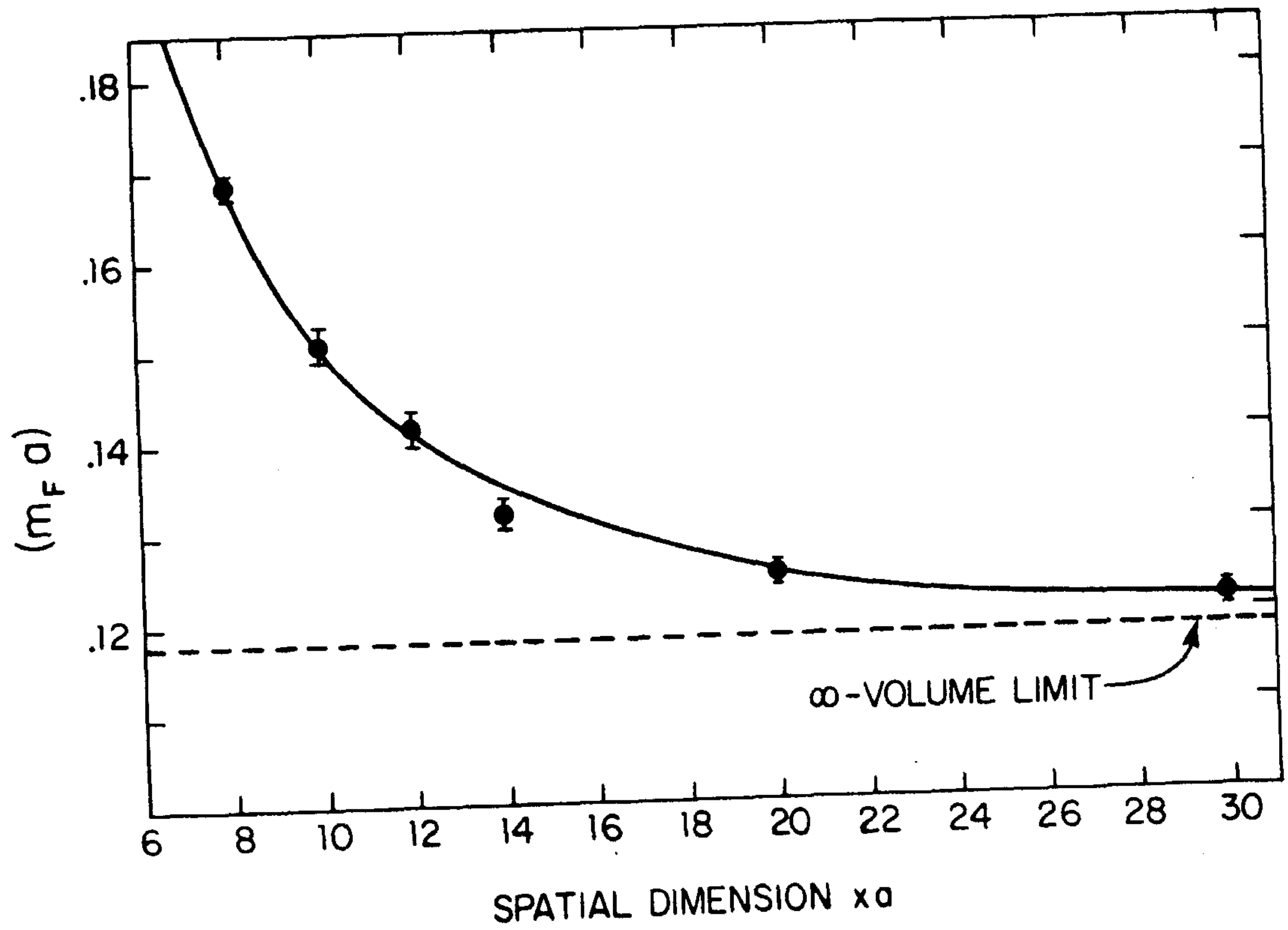


Fig. 1


.18
.16
.14
.12
(m_F a)
6
8
10
12
14
16
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20
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24
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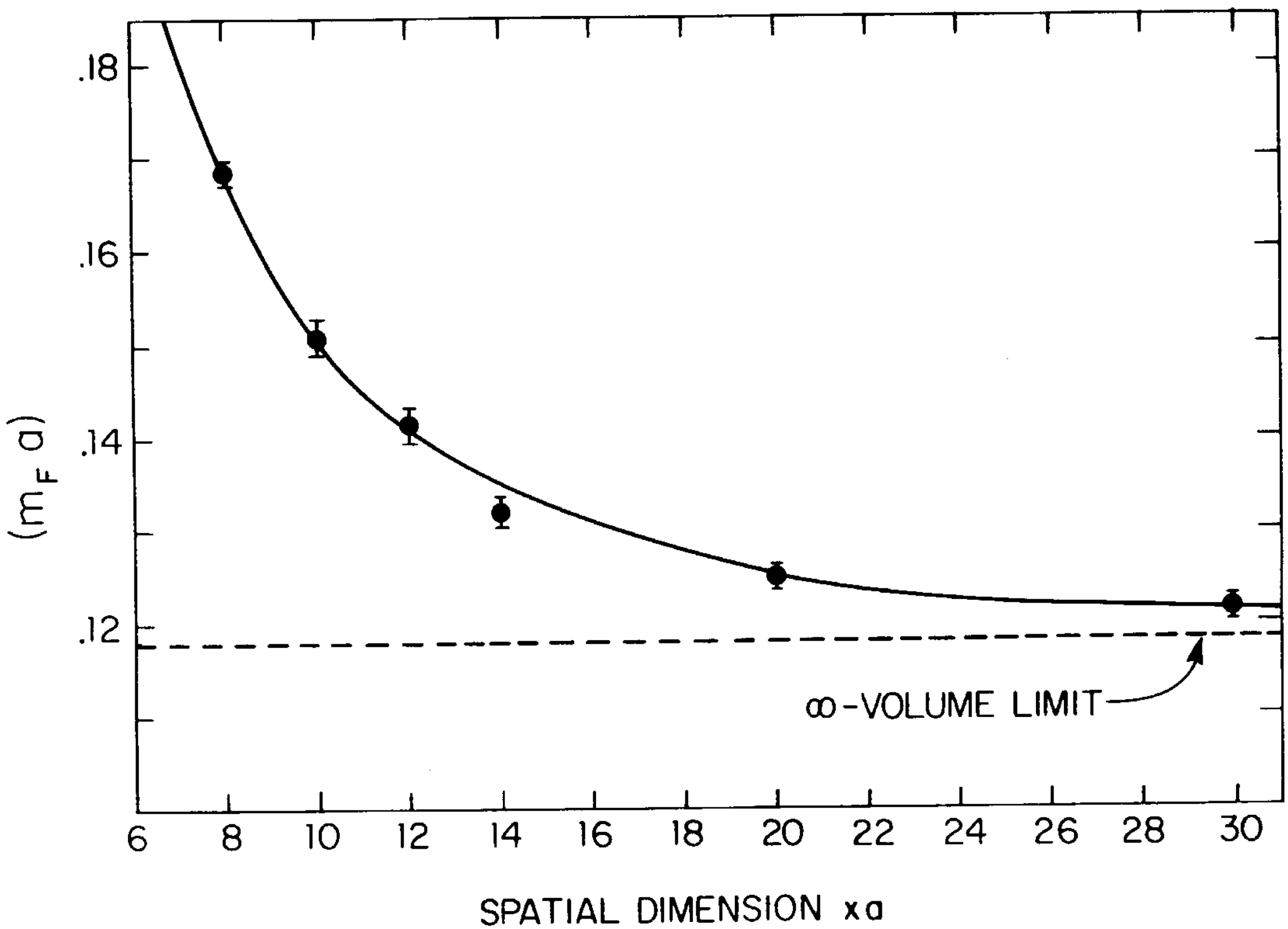
28
30
SPATIAL DIMENSION xa
∞-VOLUME LIMIT

Fig. 2



(m_F a)
.18
.16
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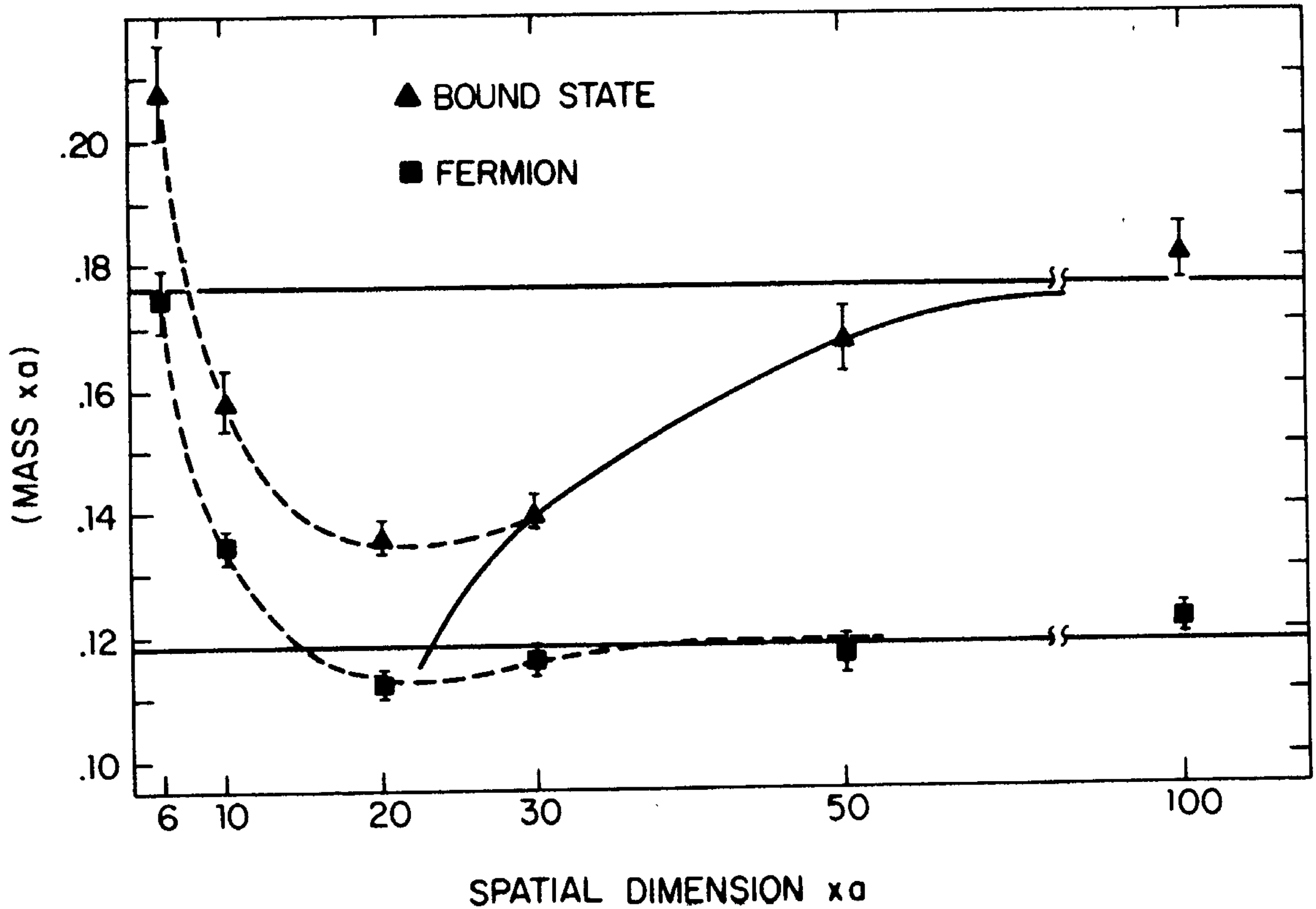
∞-VOLUME LIMIT
SPATIAL DIMENSION xa



BOUND STATE
FERMION
.20
.18
.16
.14
.12
.10
(MASS x a)
6
10
20
30
50
100
SPATIAL DIMENSION x a

Fig. 3

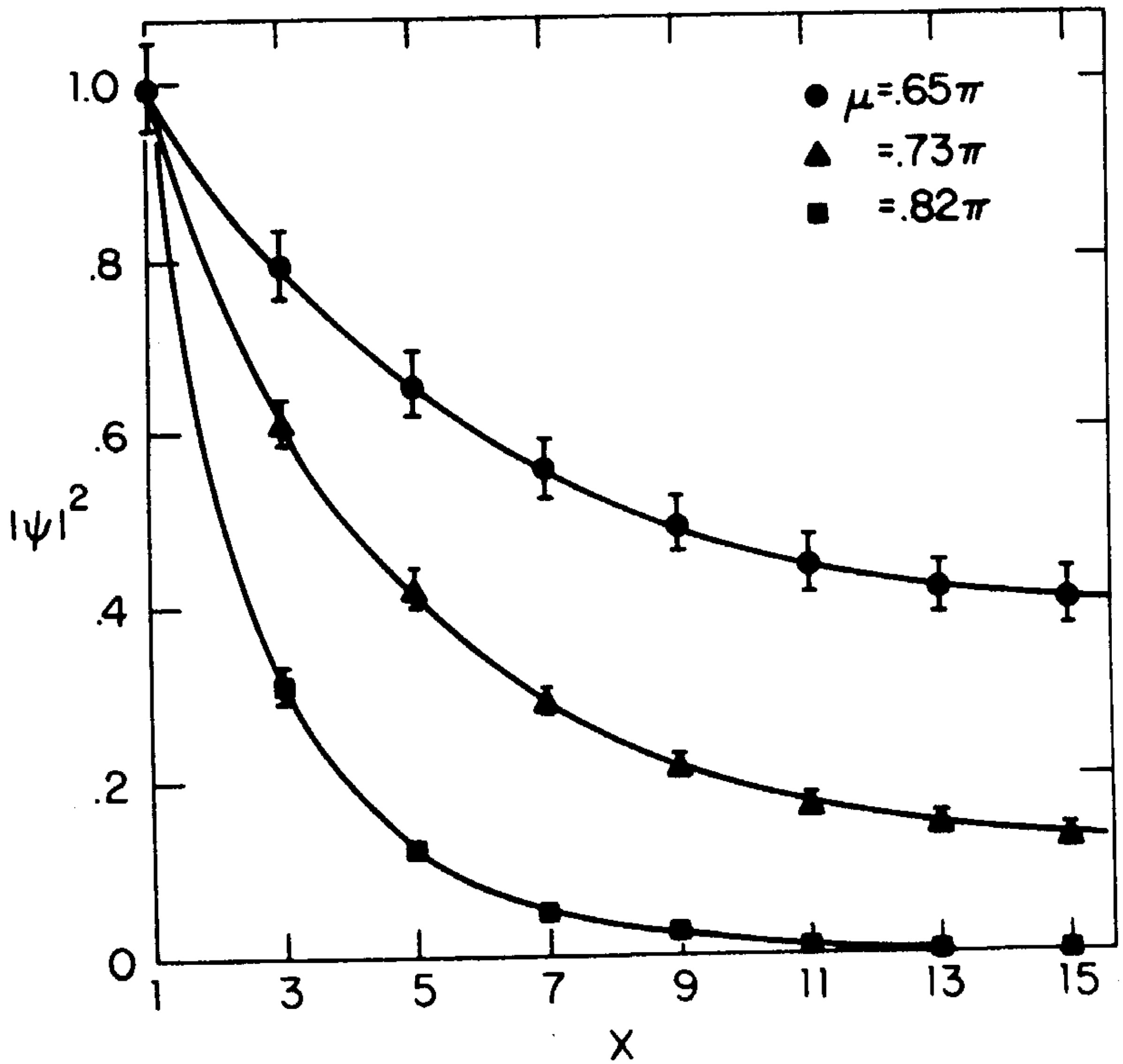


Fig. 4